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Solid solution of $CaSiO_3$ and $MgSiO_3$ perovskites in the lower mantle: The role of ferrous iron

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Abstract

The solid solution between $CaSiO_3$ and $MgSiO_3$ perovskites is an important control on the properties of the lower mantle but the effect of one of the most important impurity elements (iron) on this solution is largely unknown. Using density functional theory (DFT), ferrous iron's influence on the reciprocal solubility of $MgSiO_3$ and $CaSiO_3$ perovskite (forming a single Ca-Mg mixed perovskite phase) was calculated under pressures and temperatures of 25–125 GPa and 0–3000 K, respectively. Except at iron-rich conditions, ferrous iron preferentially partitions into the mixed perovskite phase over bridgmanite. This is a small effect (partitioning coefficient K_D ~0.25–1), however, when compared to the partitioning of ferrous iron to ferropericlase, which rules out perovskite phase mixing as a mechanism for creating iron-rich regions in the mantle. Iron increases the miscibility of Ca and Mg perovskite phases and reduces the temperature at which the two perovskite phases mix but this effect is highly nonlinear. We find that for a pyrolytic mantle [Ca% = 12.5 where Ca% = Ca/(Ca+Mg)] a perovskite ferrous iron concentration of ~13% leads to the lowest mixing temperature and the highest miscibility. With this composition, 1% ferrous iron in a pyrolytic composition would lead to mixing at ~120 GPa along the geothermal gradient, and 6.25% ferrous iron leads to mixing at ~115 GPa and 13% ~110 GPa. At high iron concentrations, Fe starts to impair miscibility, with 25% ferrous iron leading to mixing at ~120 GPa. Thus, in normal pyrolytic mantle, iron could induce a small amount of Ca-pv and Mg-pv mixing near the D″ layer but it generally partitions to ferropericlase instead and does not impact mixing. Extremely iron rich parts of the lower mantle such as ULVZs or the CMB (potentially) are also not a likely source of phase mixed perovskites due to the nonlinear effect of ferrous iron on phase mixing.

Keywords: $CaSiO_3$, $MgSiO_3$, iron, miscibility, the lower mantle; Physics and Chemistry of Earth's Deep Mantle and Core